

Topological Character of Excitations in Strongly Correlated Electronic Systems: Confinement and Dimensional Crossover.

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Abstract

Topologically nontrivial states are common in symmetry broken phases at macroscopic scales. Low dimensional systems bring them to a microscopic level where solitons emerge as single particles. The earliest and latest applications are conducting polymers and spin-Peierls chains. After a history introduction, we shall discuss the topological aspects of elementary excitations, especially the confinement and the dimensional D crossover. At the $1D$ level we exploit results of different exact and approximate techniques in theory of solitons, for both quantum and semiclassical models, and the related knowledge on anomalous charges and currents. At higher D the topological requirements for the combined symmetry originate the spin- or charge- roton like excitations with charge- or spin-kinks localized in the core. In quasi $1D$ world they can be viewed as resulting from a spin-charge recombination due to the $3D$ confinement.

1 History Introduction.

This publication is not a regular article but rather a script of the recent talk at [1], p. 169, with extensions from the one at [2]. Thus there will be no systematic references except for reviews, but I shall try to remind the names. Self-references on related publications can be found at the author's web site. The historical part² is guided by real time observations since three decades which differ from contemporary views. The original part is largely unpublished: it was developed through a sequence of talks starting from the lecture at [3]. First will be an excursion to a relevant history of interacting fermions in quasi one-dimensional $-1D$ systems. Topics on solitons and their origin will follow: classical, quasi-classical and quantum models, relations to field theory; $1D$ features - anomalous charge, spin, currents, nontrivial topology. Finally we shall come to the goals - problems at higher dimensions $D > 1$: confinement, topological constraints, combined symmetry, spin-charge recombination.

The discovery of Organic Superconductivity by Bechgaard, Jerome and Ribault was indeed a long awaited D-day of landing. Among many earlier efforts in chemistry and experiments, this anniversary recalls also the history of theories

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² A specific for the anniversary discussion of [1] is shortened in the present version.

for interacting electrons in (quasi) 1D systems. The roots hide deep in decades winding through works of Bethe, Bloch, Fröhlich, Peierls, Tomonaga. The stem emerged some three decades ago, largely nourished by the Little idea of a High- T_c superconductivity in hypothetical chain compounds. The three major lines were opened at once: Bethe Ansatz exact solutions – Gaudin, Lieb & Wu; Bosonization – Luttinger, Mattis & Lieb, Luther & Emery; Parquet Equations (an old form for the later renormalization group RG) – from Bychkov, Gor’kov & Dzyaloshinskii till Dzyaloshinskii & Larkin and Solyom *et al.* By late 70’s the prophets have left the field leaving for us the Old Testament ([4], [5]) which later became obsolete and by now abandoned in favor of New ones. Nowadays only a semantics like the *g-ology* reminds this breakthrough epoch.

Physics of microscopic solitons is a late branch of theoretical studies in 1D models. It was endorsed by high expectations from non perturbative methods and by general interests in topologically nontrivial configurations, e.g. [6, 7], see more refs. in [9]. First were classical models with degenerate ground states (Bishop, Krumhansl, Rice, Schrieffer, *et al.*). Largely the studies were stimulated by first observations of Charge Density Waves -CDW’s (Comes, Pouget, Shirane *et al.*) and especially by discovery of their sliding (Monceau & Ong) where effects of commensurate versus incommensurate (C, IC) states seemed to be important³. An impact came also from the field theory where quasi classical solitonic solutions of multi-electronic Gross-Neveu type models were discovered (Neveu *et al.*, Fateev). The multi-electronic theory of adiabatic models (Peierls, Fröhlich) in applications to CDW/SDW was developed [10, 11, 12]. A very popular discrete version of the Peierls model is known as the Su-Schrieffer-Heeger one [13, 14], in which frame much numerical work on solitons have been performed. A surprise from these models with seemingly well behaved normal electronic spectra in the ground state was that their excited states developed spin-charge and spectral anomalies [10]. It was a consequence of electronic selftrapping to topologically nontrivial forms: amplitude and mixed solitons. The discovery of doped polymers has triggered an avalanche of experimental (especially initiated by Heeger *et al.*) and related theoretical (Schrieffer *et al.*, S.B.-Kirova-Matveenko; Bishop & Campbell, Maki *et al.*, Yu Lu *et al.*) studies on solitons, see reviews [10, 13, 14]. The key words were solitons, polarons, bipolarons, mid-gap states, pseudo-gap, etc.

The contribution from our place was initially provoked by the problem, posed that time by Lee, Rice and Anderson, of a pseudo-gap⁴ Largely the studies were based on finding exact solutions for major basic models and later on realizing the confinement problem. We benefited from the field theory results (Neveu *et al.*, Fateev) and from special mathematical methods (Dubrovin & Novikov, Krichever). On this way the solitonic solutions were generalized to multiple quasi periodic structures allowing to describe a simultaneous effect of the doping and the spin (or interchain) splitting⁵ or the effect of lattice discreteness, a spill-

³ As a solitonic lattice the slightly IC state has been first described by Dzyaloshinskii for magnetic media. Later it was rediscovered several times, e.g. for CDWs.

⁴ An essential part of these results (S.B. & Dzyaloshinskii 76, S.B. 78,80) have been recently republished, in a striking similarity, by the Ohio-Australia group but unfortunately only one side of the old studies have been captured. The missing link is a division of characteristic time scales: fast like in Optics and PES against slow like in kinetics and thermodynamics. Only the fast ones are relevant for electronic pseudo gaps while the slow ones must be signatures of either collective modes or of associated solitons [12].

⁵ This theory is a route to current studies of spin-Peierls systems in high magnetic fields

over formation (S.B., Gor'kov and Schrieffer) of superlattices due to electronic 3D dispersion. Finally the quantization of solitons was performed in these multi fermionic models (S.B. & Matveenko 89) showing new anomalous currents.

A fully quantum approach to solitons have been called earlier when an equivalence had been found between models of interacting electrons, Sine-Gordon and Coulomb gas, see e.g. [15]. The most powerful tool became the Bosonization, see e.g. the recent book [16], especially after the Luther & Emery work. It allowed to access explicitly the spin-charge separation, to refine the form of the Green functions - logarithmic corrections upon the Dzyaloshinskii-Larkin scaling solution (Finkelstein), etc. Both the RG and exact Bethe Ansatz solutions (Nersessyan & Wiegman) of the quantum Sine Gordon model have been employed, providing the quantum description of the C-IC transition.

With solitons being inhabitants of the 1D underground, the questions were risen (S.B. 1980): Can they cross the boarder to the higher D world? If yes, then are they allowed to bring their anomalies? A password was found - a *confinement*: as topological objects (see [9] for references) connecting the degenerate vacuums, the solitons at $D > 1$ acquire an infinite energy unless they reduce or compensate their topological charges.

Here we can notice a similarity in histories of solitons and of interacting electrons with respect to entering the higher dimensional world. In both cases a long staying and still practicing belief is that the exotic 1D properties will be maintained which is far from being correct in general. For solitons this is a devastating effect of the confinement (S.B. 80). For electrons this is a decoherence of their interchain hopings which erases the memory of 1D correlations in the gapless (the Luttinger Liquid of later days) regime (S.B. and Yakovenko 85).

2 Confinement and combined excitations.

2.1 A quasi classical commensurate CDW: confinement of phase solitons and of kinks.

Being a case of spontaneous symmetry breaking, the CDW order parameter $\sim \Delta \cos[\vec{Q}\vec{r} + \varphi]$ possesses a manifold of degenerate ground states. For an IC CDW the global symmetry allows for arbitrary shifts in phase φ which originates the phenomenon of sliding discovered by Monceau and Ong (recall theories by Fröhlich; Bardeen *et al*; Lee, Rice & Anderson; S.B. & Dzyaloshinskii). For an M -fold commensurate CDW the energy $\sim \cos[M\varphi]$ reduces the allowed positions to multiples of $2\pi/M$, $M > 1$. The trajectories connecting them $\varphi \rightarrow \varphi + 2\pi/M$ are the phase solitons -PSs, or " φ - particles" after Bishop *et al*. For a special case (e.g. in the conjugated polymer *trans* - CH_x) of $M = 2$, the φ shift by π is replaced by an equivalent sign change of the amplitude, the kink $\Delta \rightarrow -\Delta$. It matches the existence of amplitude solitons -ASs even for the IC CDW without the topological selection (S.B. 78). If the system is 1D, or at least it is above the 3D or 2D transition temperature T_c , then the local symmetry coincides with the global one. In these regimes the symmetry is not broken and the solitons are allowed to exist as elementary particles. But in the symmetry broken phase at $T < T_c$, any local deformation must return the system to the same,

(Berthier et al, Boucher & Regnault in [17] p. 1939, Poilblanc et al), especially if extended to doped case.

or equivalent (modulo 2π), state. Otherwise the interchain interaction energy (with linear density $F \sim \langle \Delta_0 \Delta_n \cos[\varphi_0 - \varphi_n] \rangle$) is lost when the effective phase $\varphi_0 + \pi \text{sign}(\Delta_0)$ at the soliton bearing chain $n = 0$ acquires a finite (and $\neq 2\pi$) increment with respect to the neighboring chain values φ_n . The 1D allowed solitons do not satisfy this condition which originates a constant *confinement force* F between them, hence the infinitely growing confinement energy $F|x|$. E.g. for $M = 2$ the ASs should be *bound to pairs of kinks*; for an arbitrary M the PSs should *aggregate in trains* of M solitons, thus accumulating an allowed increment 2π of the phase. For an IC CDW at $D > 1$, the local 2π solitons appear as the only allowed increments of one chain with respect to the surrounding ones. If a large number of adjacent chains acquires this increment coherently, then one can recognize the dislocation loop -DL embracing this bundle (Dumas, Feinberg, Friedel; S.B. and Matveenko). The aggregation of solitons into minimal allowed complexes is expected for high T versus low concentration, for impurities trapping or due to long range Coulomb interactions. For a pure system and at low T , when the entropy plays no more role, the solitonic complexes should aggregate into macroscopic objects, the bubbles. They are encircled by the lines which are relevant to DLs in IC systems. But instead of the homogeneous 2π circulation of the phase around the DL, the bubble boundary emits the M surfaces (stripes) each providing the $2\pi/M$ phase jumps, just as it has been observed by Chen *et al.* When the bubbles extends to the sample width, the plains decouple into unbound Domain Walls separating domains with different global values of the order parameter. It was found (S.B. & T.Bohr) that the crossover between the aggregation due to the confinement and the size effect applies to 2D systems only. In 3D a second phase transition of an infinite aggregation should be expected.

In summary, here are the known scenarios for the deconfinement:

Aggregation versus thermal deconfinement (S.B. & T.Bohr 83);

Coupling of kinks to structural topological defects - twistons in polymers
(S.B. & Kirova 88,91,92);

Binding into kink-antikink pairs and the origin of bipolarons
(S.B. & Kirova 81);

A compensation by gapless degrees of freedom: the *today's specialty*.

2.2 A quasi classical CDW: confinement of Amplitude Solitons with phase wings.

The CDW order Parameter is $O_{cdw} \sim \Delta(x) \cos[Qx + \varphi]$ where Δ is the amplitude and φ is the phase. In 1D the ground state with an odd number of particles contains the AS $\Delta(x = -\infty) \leftrightarrow -\Delta(x = \infty)$, Figure 1. It carries the singly occupied mid-gap state, thus having a spin 1/2 but its charge is compensated to 0 (fractional variable charges also appear at circumstances) by local dilatation of singlet vacuum states. As a nontrivial topological object (O_{cdw} does not map onto itself) the pure AS is prohibited in $D > 1$ environment. Nevertheless it becomes allowed in $D > 1$ if it acquires phase tails with the total increment $= \pi$, Figure 2. The length of these tails ξ_φ is determined by a weak interchain coupling, thus $\xi_\varphi \gg \xi_0$. As in 1D, the sign of Δ changes within the scale ξ_0 but

further on, at the scale ξ_φ , the sign of the factor $\cos[Qx + \varphi]$ also changes the sign thus leaving the product in O_{cdw} to be invariant. As a result the 3D allowed particle is formed with the AS core $\xi_0 \sim 10\text{\AA}$ carrying the spin and the phase $\pi/2$ twisting wings $\xi_\varphi \sim 100\text{\AA}$, each carrying the charge $e/2$. Nevertheless the spin-charge reconfinement is not the end of the story. When the combined soliton moves, its locale electric current is compensated exactly by the back flow currents at distant chains. This is the property of the vortex like configuration. Finally, the a soliton as a state of the coherent media will not carry a current and himself will not be driven by a homogeneous electric field. But locally, e.g. interacting with a charge impurity, it will behave as a charged particle. This paradox can be proved as a theorem (S.B. 80) for a general system with electronic interactions. We shall return to this property below.

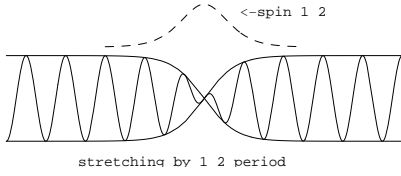


Figure 1: An amplitude soliton in the IC CDW

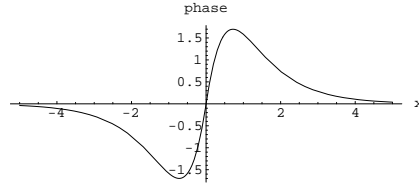


Figure 2: Phase tails (between 0 and $\pi/2$) adapting the AS.

2.3 Quantum models based on bosonization.

2.3.1 A hole in the AFM environment.

Consider first the quasi 1D system with repulsion at a nearly half filled band which is the Spin Density Wave -SDW route to a general doped antiferromagnetic -AFM Mott-Hubbard insulator. The bosonized Hamiltonian (Luther & Emery) can be written schematically (*numerical coefficients are not shown, only terms relevant to repulsion are left*) in 1D as

$$H_{rep} \sim \{(\partial\varphi)^2 - U\cos(2\varphi)\} + (\partial\theta)^2$$

where φ is the analog of the CDW displacement phase and θ is the angle of the $SU2$ spin rotation. Here U is the Umklapp scattering amplitude of Luther & Emery (or g_3 of Dzyaloshinskii & Larkin) which is a feature of systems with a single mean occupation of lattice sites. Normally U is of the order of other interactions which are not small. Hence a big gap is opened in the charge φ - channel so that only gapless spin degrees of freedom are left for observations. But a generous feature of just the Bechgaard salts⁶ is that $U \sim g_3$ is small appearing only as a secondary effect of the anionic sublattice. It opens an intriguing crossover

⁶ This feature was noticed in the very first work (S. Barisić and S.B. 81) done in response to the D-day which was a natural application of the recently having been developed (S.B. and S. Gordyulin, 80) concept of the "weak two-fold commensurability". Even more intriguing manifestations of various types of anions' ordering have been noticed and analyzed (S.B. and V. Yakovenko 85) after systematic structural studies became available (see J.-P. Pouget review talk in [1] and, with S. Ravy, in [17]).

Figure 3: An illustration of the hole motion in the AFM media accompanied by the rotation of spins. The string of the reversed AFM order created by the holon is cured by the semi-vortex of the staggered magnetization. The same figure is applied to the below case of the superconductivity with lines of electric currents instead of contours of spin rotations and with the spin carrying normal core instead of the moving hole.

Now it is straightforward to build a universal formulation which extends to isotropic AFM systems like the CuO_2 planes. The SDW is now a staggered magnetization, the soliton becomes a hole moving within the AFM environment, the π wings become the magnetic semi-vortices (see [9] for a macroscopic illustration). The resulting configuration is a half-integer vortex ring of the staggered magnetization (a semi roton) with the holon confined in its center, Figure 3. (In $2D$ the vortex ring is reduced to the pair of vortices.) The solitonic nature of the holon in quasi $1D$ corresponds to the string of reversed staggered magnetization (Nagaev *et al*, Brinkman and Rice) left by the moving hole (see [18] for the latest review). This approach allows to calculate the physical variables like the localized charge, the delocalized staggered spin density S_{afm} and the net (ferromagnetic) magnetization S_{fer} , the corresponding currents, etc. E.g. at large distances we have⁷ $S_{afm} \sim x/(x^2 + y^2)$ where x is the motion direction. The induced non oscillating magnetization is

$$S_{fer} \approx \delta(x)\delta(y) + \frac{1}{2\pi}(x^2 - y^2)/(x^2 + y^2)^2$$

Here the first term comes from the single spin density localized in the wings of the combined core around the charged nucleus. The second term is the counter rotation of the staggered magnetization at distant chains. The coefficients of these terms are fixed and correlated in such a way that, being integrated over the cross-section y , the two contributions cancel each other *identically in x* .⁸ This

⁷ There is a typing mistake in the corresponding formula in [1].

⁸ To deal correctly with shape dependent dipole distribution, the prescription is to interpret the last term as $\sim \partial_x[x/(x^2 + y^2)]$ which invokes the semiroton as the origin of long range distortions.

cancellation, in addition to the combined core properties, is a new information in addition to the spin wave theory results of Shraiman and Siggia. It opens an important paradox already mentioned above for CDW: integrally the spin current of the moving particle is transferred to the collective mode of a homogeneous rotation leaving only the charge current as for the holon in 1D. But locally, via NMR e.g., it will be seen as the nominal electronic spin. Thus in quasi-1D picture, following the path of the soliton bearing chain, the normal local quantum numbers are found: spin $s = 1/2$ (while in wings) and charge $e = 1$ (while in the core).

2.3.2 Spin-Gap cases: the quantum CDW and the superconductivity.

For systems with attraction between electrons the bosonized Hamiltonian reads

$$H_{atr} \sim \{(\partial\theta)^2 - V\cos(2\theta)\} + (\partial\varphi)^2$$

where V is the backward exchange scattering (Luther & Emery, g_1 of Dzyaloshinskii *et al*, see Gor'kov in [17]). The Umklapp term of the earlier H_{rep} is either absent for an IC case or renormalized to zero, in a similar way as it was for V in the repulsion case. The elementary excitations at 1D are the *spinon* as a soliton $\theta \rightarrow \theta + \pi$ and the gapless charge sound in φ .

The CDW order parameter is

$$O_{cdw} \sim \Psi_{+\uparrow}^+ \Psi_{-\uparrow} + \Psi_{+\downarrow}^+ \Psi_{-\downarrow} \sim \exp[i(Qx + \varphi)] \cos \theta$$

Hence for the CDW ordered phase in a quasi 1D system the allowed configuration is composed with the spin soliton: $\theta \rightarrow \theta + \pi$ and the wings $\varphi \rightarrow \varphi + \pi$ where the charge $e = 1$ is concentrated. Beyond a low dimensionality, a general view is: the *spinon as a soliton bound to the semi-dislocation loop*. The same paradox is observed as for the classical CDW and similar to the AFM cases: locally the single electronic quantum numbers are reconfined (while with different scales of localization); but integrally still there is only the moving spin while the charge is transferred to the collective sliding mode.

For the singlet superconductivity SC the order parameter is

$$O_{sc} \sim \Psi_{+\uparrow} \Psi_{-\downarrow} + \Psi_{+\downarrow} \Psi_{-\uparrow} \sim \exp[i\tilde{\varphi}] \cos \theta$$

where the gauge phase $\tilde{\varphi}$ is conjugated to the chiral one φ - the last term in H_{atr} can be written reciprocally as $\sim (\partial\tilde{\varphi})^2$ as well (Efetov & Larkin). In $D > 1$ the elementary excitation is composed by the *spin soliton* $\theta \rightarrow \theta + \pi$ supplied with *current wings* $\tilde{\varphi} \rightarrow \tilde{\varphi} + \pi$. A quasi 1D interpretation is that the *spinon works as a Josephson π - junction* in the superconducting wire. The 2D view is a pair of superconducting π - vortices sharing the common core where the unpaired spin is localized. The 3D view is a half flux vortex loop which collapse is prevented by the spin confined in its center.

In summary of this chapter notice that the factorization of typical order parameters reflects the combined global symmetry of the ordered phase, e.g. for the AFM, SDW this is a product of translations and the time reversal (S.B. and I. Luk'yanchuk 89-91). Beyond applications to solitons, it affects other observable physical properties dependent on spin-charge reconciliation. Thus, the optical absorption across the spin gap becomes allowed contrary to the basic models (S.B. and A. Finkelstein 81).

3 Conclusions.

The discovery of the organic superconductivity with its striking proximity to the AFM phase has changed the accents of theories from the earlier dominated Little model of strong on-chain attraction to the ones with repulsion and the related Mott-Hubbard insulator phase. Adding the later studies on the interchain electronic coupling/coherence we see that the major problematics of the High- T_c epoch has been risen years in advance. Later on the theory of 1D electronic systems has been called to elucidate the hypotheses risen in High- T_c epoch (P.W. Anderson). Here we have explored this opportunity once again in some other aspects. Thus the slightly IC SDW can be viewed as a prototype of the doped AFM, etc. Exploiting another analogy, to quarks and gluons in QCD, separate spinons and holons are not observed directly because of the topological confinement. The topological effects of $D > 1$ ordering reconfines the charge and the spin *locally* while still with essentially different distributions. Nevertheless *integrally* one of the two is screened again, being transferred to the collective mode, so that in kinetics the massive particles carry only either charge or spin again.

Acknowledgments. I recall a great fortune of collaborations on above subjects with S. Barisic, T. Bohr, I. Dzyaloshinskii, A. Finkelstein, L. Gor'kov, N. Kirova, I. Krichever, A. Lebed, S. Matveenko, Ph. Nozieres, J.R. Schrieffer and V. Yakovenko.

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